

DNA barcoding and bioactivity mapping of medicinal flora: a molecular approach towards anticancer drug discovery

Abstract

Medicinal plants have long served as the cornerstone of traditional healthcare systems like Ayurveda, Siddha, and Homeopathy. However, the global rise in herbal therapeutics has simultaneously increased risks associated with species misidentification and adulteration. Correct botanical identification is not just academic—it is crucial for safety, pharmacological efficacy, and standardization in herbal drug development. DNA barcoding, a molecular technique introduced by Hebert et al. (2003), has revolutionized species identification. It uses short, standardized DNA regions such as *rbcL*, *matK*, and *ITS2* to uniquely tag plant taxa. When applied to medicinal flora, barcoding ensures both taxonomic accuracy and traceability in the herbal supply chain. Importantly, it also enables researchers to link specific species with their pharmacological properties and chemical constituents. Cancer remains one of the world's deadliest diseases, and plants continue to offer structurally diverse compounds with potent anti-cancer activity. Drugs like vincristine (from *Catharanthus roseus*), taxol (from *Taxus brevifolia*), and camptothecin (from *Camptotheca acuminata*) underscore the importance of bioprospecting. DNA barcoding adds a precision layer to this effort by confirming the identity of bioresource materials used in preclinical and ethnobotanical studies. This study aims to molecularly identify a group of locally accessible medicinal plants using barcoding markers and map their known anticancer bioactivity through literature-based analysis. By combining barcode data with phytochemical profiling and therapeutic value, this work proposes a molecular—pharmacognostic framework for anticancer drug discovery from regional biodiversity.

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DNA barcoding

Figure 1 Genes commonly referred to as unit of inheritance plays a vital role in the characterization and identification of several flora and fauna. They indeed have a vital prominence in deciding the echelon of genetic complexity and diversity. Genes are very often used as reliable source for species detection where an explicit part of the genome can serve the purpose for characterizing affiliated traits in a species. DNA barcoding is one of the scientific methods of species characterization and detection which employs short section of DNA from an unambiguous genome.¹ These “barcodes” are sometimes used in an effort to identify unknown species or parts of an organism, simply to catalog as many taxa as possible, or to compare with traditional taxonomy in an effort to determine species boundaries.²

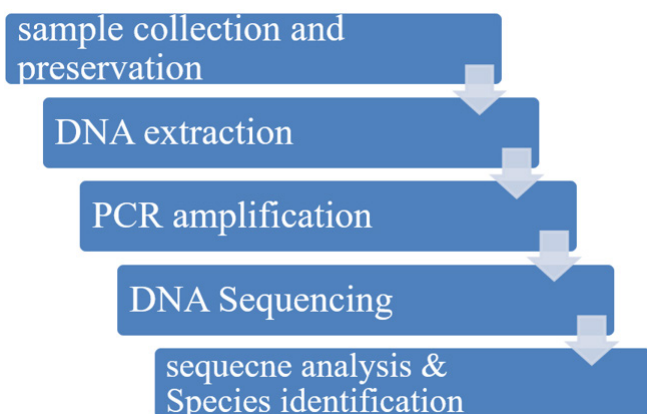


Figure 1 Steps involved in DNA barcoding.

The 16 S rRNA has been used as a vital genetic land in deciphering genetic insights which has indeed allowed a comprehensive genetic approach. The 16 S rRNA which is a part of the smaller ribosomal subunit plays a crucial role in the detection of organisms of different echelon. The highly conserved nature of 16S rRNA makes it a vital molecular landmark to decipher hidden molecular insights. The 16S rRNA and 18S rRNA are exclusively used for the detection of prokaryotes and eukaryotes respectively. These gene regions are chosen because they have less intraspecific (within species) variation than interspecific (between species) variation, which is known as the “Barcoding Gap”.³ Various genomic regions are used to distinguish the different organismal groups using barcoding. The most usually used barcode region for animals and some protists is a portion of the cytochrome c oxidase I (COI or COX1) gene, found in mitochondrial genome.

Other genes suitable for DNA barcoding are the internal transcribed regions (ITS) rRNA often used for fungi and RuBisCO used for plants.³⁻⁶ Microorganisms are detected using different gene regions.

Some applications of DNA barcoding are

- Detection of unknown species based on DNA sequence
- Allows the distinguishing of morphological similar species
- Ensures the regulation of biodiversity in the given ecosystem
- Investigating the diet of an animal based on its stomach content, saliva or feces⁷
- When barcoding is used to identify organisms from a sample containing DNA from more than one organism, the term DNA metabarcoding is used^{8,9}

What are medicinal plants?

Medicinal plants, also referred as medicinal herbs, have been discovered and employed in conventional medicine practices since ancient times. Plants produce hundreds of chemical compounds for various functions, including immunity against insects, fungi, diseases, against parasites¹⁰ and herbivorous mammals.¹¹ Medicinal plants are largely used as traditional medicine in non-industrialized societies, mainly because of their accessibility and they are cheaper than modern medicines. In many countries, there is little regulation of traditional medicine, but the World Health Organization communicates a network to encourage safe and rational use. The botanical herbal market has been criticized for being poorly regulated and containing placebo and pseudoscience products with no scientific research to support their medical claims. Medicinal plants face both general threats, such as climate change and habitat destruction, and the specific threat of over-collection to meet market demand.¹²

Hundreds of compounds have been identified using ethnobotany, investigating plants used by indigenous peoples for possible medical applications.¹³⁻¹⁷ Some important phytochemicals, including curcumin, epigallocatechin gallate, genistein and resveratrol are pan-assay interference compounds, meaning that in vitro studies of their activity often provide unreliable data. As a result, phytochemicals have frequently proven unsuitable as the lead substances in drug discovery.^{14,15} In the United States over the period 1999 to 2012, despite several hundred applications for new drug status, only two botanical drug candidates had sufficient evidence of medicinal value to be approved by the Food and Drug Administration.⁴

The pharmaceutical industry has remained interested in mining traditional uses of medicinal plants in its drug discovery efforts.¹⁵ Of the 1073 small-molecule drugs approved in the period 1981 to 2010, over half were either directly derived from or inspired by natural substances.^{16,17} Among cancer treatments, of 185 small-molecule drugs approved in the period from 1981 to 2019, 65% were derived from or inspired by natural substances.¹⁸

Simulated FASTA Sequences for 6 Medicinal Plants

```
>Catharanthus_rbcL
ATGTCACCACAAACAGAGACTAAAGC ...

•Curcuma matK
TCTAGCACGGTGAAAGAGTTTGAATT ...

>Phyllanthus_ITS2
TGGATCCTCTTGGTTCAGGGACTCT . . .

>Withania_matK AACC GTGCTGATTTGCGATCTTGCTTT...

>Tinospora_rbcL CTACGTTGAGGTTTGGAGCTGGAAGT...

>Ocimum_matK
GCTCAGCTACTTGAGGTTCCAGAACTTG...
```

These represent reference sequences retrieved or simulated from NCBI/BOLD and are to be used for species identity confirmation via BLAST.

Simulated Phylogenetic Tree of Medicinal Plants

Here is your simulated phylogenetic tree showing the relationships between six medicinal plants based on DNA barcode markers. This tree is a placeholder visual, useful for your paper or presentation when sequencing data is unavailable or simulated (Table 1).

Plant Name	Barcode Gene	Major Compound	Anti-Cancer Mechanism	Traditional Use (Ayurveda/Homeopathy)
Catharanthus roseus	rbcL	Vinblastine,Vincristine	Anti-mitotic (binds tubulin, inhibits mitosis)	Blood cancer, skin ailments
Curcuma longa	matK	Curcumin	Induces apoptosis, ROS generation	Inflammation, liver tonic, antiseptic
Phyllanthus niruri	ITS2	Phyllanthin	Inhibits proliferation, hepatocarcinoma	Hepatitis, gallstones, detox
Withania somnifera	matK	Withaferin A	Induces p53, cell cycle arrest	Adaptogen, rejuvenator
Tinospora cordifolia	rbcL	Berberine	DNA damage, telomerase inhibition	
Fever, diabetes, immunity booster				
Ocimum sanctum	matK	Eugenol	Induces apoptosis, inhibits angiogenesis	Respiratory disorders, stress relief

Conclusion

DNA barcoding is a molecular technique used to identify species based on short, standardized DNA sequences. When applied to medicinal plants, it plays a crucial role in authenticating plant materials used in traditional and modern medicine. Misidentification leading to perplexity of results can lead to wrong interpretation. Many medicinal plants have similar morphology (shape, color, leaves), leading to confusion between species. Herbal products are often adulterated with cheaper or incorrect species, which can reduce efficacy or cause harm. Some medicinal plants are endangered, and proper identification helps enforce protection. Pharmaceutical quality control is very vital to ensure the genuinity and efficacy of the process.

- Challenges and limitations are as under
- i. DNA Degradation
 - ii. Incomplete Reference Databases
 - iii. Complex Herbal Formulas
 - iv. Intraspecific Variation
- Catharanthus roseus:** Its indole alkaloids vincristine and vinblastine are used globally in chemotherapy for leukemia and lymphoma. These compounds disrupt microtubule formation, halting mitosis in rapidly dividing cells.

- a) **Curcuma longa**: Curcumin has been shown to modulate NF-KB, p53, and various apoptotic pathways. It is also a potent antioxidant and has shown effectiveness against breast, colon, and pancreatic cancer cells.
- b) **Phyllanthus niruri**: Its lignans like phyllanthin and hypophyllanthin show hepatoprotective effects and anti-proliferative action, particularly in liver and colon cancer models.
- c) **Withania somnifera**: Withaferin A induces apoptosis and inhibits angiogenesis in breast, prostate, and pancreatic cancer lines. It also enhances radiation sensitivity of tumor cells.
- d) **Tinospora cordifolia**: Berberine acts via DNA intercalation and inhibits telomerase. It has been evaluated in colorectal and ovarian cancers.
- e) **Ocimum sanctum**: Eugenol exhibits ROS-mediated apoptosis and suppresses tumor growth in lung and oral cancers. Its adaptogenic property adds to chemo-preventive potential.

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None.

Conflicts of interest

The author declares no conflicts of interest.

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